

# Theory of magnetic order in the three-dimensional spatially anisotropic Heisenberg model

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A spin-rotation-invariant Green's-function theory of long-range and short-range order (SRO) in the  $S = 1/2$  antiferromagnetic Heisenberg model with spatially anisotropic couplings on a simple cubic lattice is presented. The staggered magnetization, the two-spin correlation functions, the correlation lengths, and the static spin susceptibility are calculated self-consistently over the whole temperature region, where the effects of spatial anisotropy are explored. As compared with previous spin-wave approaches, the Néel temperature is reduced by the improved description of SRO. The maximum in the temperature dependence of the uniform static susceptibility is shifted with anisotropy and is ascribed to the decrease of SRO with increasing temperature. Comparing the theory with experimental data for the magnetization and correlation length of  $\text{La}_2\text{CuO}_4$ , a good agreement in the temperature dependences is obtained.

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## I. INTRODUCTION

The magnetic properties of spatially anisotropic antiferromagnetic (AFM) quantum spin systems, such as the quasi-two-dimensional (2D) parent compounds of high- $T_c$  superconductors (e. g.  $\text{La}_2\text{CuO}_4$ ,  $\text{Ca}(\text{Sr})\text{CuO}_2$ )<sup>1</sup> and the quasi-1D cuprates  $\text{Sr}_2\text{CuO}_3$ ,  $\text{Ca}_2\text{CuO}_3$ ,<sup>2,3</sup> and  $\text{SrCuO}_2$ ,<sup>4</sup> are of current interest. The main problem is the influence of spatial anisotropy on the staggered magnetization  $m$  and the Néel temperature  $T_N$  in the 3D spin- $\frac{1}{2}$  AFM Heisenberg model

$$H = J_x \left[ \sum_{\langle ij \rangle_x} \mathbf{S}_i \mathbf{S}_j + R_y \sum_{\langle ij \rangle_y} \mathbf{S}_i \mathbf{S}_j + R_z \sum_{\langle ij \rangle_z} \mathbf{S}_i \mathbf{S}_j \right]. \quad (1)$$

Here  $R_y = J_y/J_x$ ,  $R_z = J_z/J_x$  (throughout we set  $J_x = 1$ ) and  $\langle ij \rangle_{x,y,z}$  denote nearest-neighbor (NN) bonds along the  $x$ -,  $y$ - or  $z$ -directions of a simple cubic lattice. For real systems, we consider  $0 \leq R_z \ll R_y \leq 1$ .

In the paramagnetic phase, there exists a pronounced AFM short-range order (SRO) which is reflected by a maximum in the temperature dependence of the magnetic susceptibility at  $T_{max}$ , where  $0.64 < T_{max} < 1.2$ .<sup>5</sup> However, the RPA spin-wave theories<sup>6,7</sup> and the mean-field theories using auxiliary-field representations (Schwinger-boson,<sup>8,9</sup> Holstein-Primakoff,<sup>10,11</sup> Dyson-Maleev,<sup>10,12</sup> and boson-fermion

representations<sup>13)</sup> which were developed for the quasi-2D model with  $R_y = 1$ , are valid only at sufficiently low temperatures. In those theories, the temperature dependent SRO is not adequately taken into account; in particular, the maximum in the magnetic susceptibility cannot be reproduced. In the chain mean-field approaches,<sup>14</sup> recently improved by spin-fluctuation corrections<sup>15</sup> which lower  $m$  and  $T_N$ , an asymmetry between intrachain and interchain correlations is introduced. As was shown in Ref. 3 on the basis of a detailed estimate of the exchange integrals for the quasi-1D cuprates using a first-principle calculation ( $\text{Sr}_2\text{CuO}_3$ :  $R_y \simeq 0.004$ ;  $\text{Ca}_2\text{CuO}_3$ :  $R_y \simeq 0.02$ ), all previous approaches overestimate both  $m$  and  $T_N$ . This deficiency is calling for a theory that provides an improved description of SRO over the whole temperature region. In Ref. 16, a spin-rotation-invariant Green's-function theory for the 2D isotropic Heisenberg and  $t$ - $J$  models was developed, which yields a good description of spin correlation functions of arbitrary range and at arbitrary temperatures. Moreover, the susceptibility maximum was obtained in good agreement with quantum Monte Carlo calculations. Applying this approach to the 2D anisotropic Heisenberg model,<sup>17</sup> the short-ranged spin correlations at  $T = 0$  are well reproduced as compared with exact diagonalization (ED) data. Accordingly, we expect such a theory to describe the SRO properties quite well also in the 3D model (1).

In this paper we extend the Green's-function approach of Refs. 16 and 17 and present a theory of AFM long-range order (LRO) and SRO for the 3D anisotropic Heisenberg model (1) (Sec. II). Thereby, the correlations along all spatial directions are described on the same footing. In Sec. III the ground state is investigated, where the magnetization and short-ranged spin correlation functions are calculated. In Sec. IV we present our finite-temperature results on the  $R_z$ -dependence of  $T_N$ ,  $m(T)$ , and of the AFM correlation lengths. Moreover, for the first time, the effects of an arbitrary spatial anisotropy on the temperature dependence of the uniform static spin susceptibility, especially on  $T_{max}$ , are investigated. The results are compared with experiments on  $\text{La}_2\text{CuO}_4$  (magnetization, correlation length, magnetic susceptibility). The summary of our work can be found in Sec. V.

## II. DYNAMIC SPIN SUSCEPTIBILITY

To determine the dynamic spin susceptibility  $\chi^{+-}(\mathbf{q}, \omega) = -\langle\langle S_{\mathbf{q}}^+; S_{-\mathbf{q}}^- \rangle\rangle_{\omega}$  by the projection method outlined in Ref. 16, we choose the two-operator basis  $\mathbf{A} = (S_{\mathbf{q}}^+, i\dot{S}_{\mathbf{q}}^+)^T$  and consider the two-time retarded matrix Green's function in a generalized mean-field approximation,  $\langle\langle \mathbf{A}; \mathbf{A}^+ \rangle\rangle_{\omega} = [\omega - \mathbf{M}'\mathbf{M}^{-1}]^{-1} \mathbf{M}$  with  $\mathbf{M} = \langle[\mathbf{A}, \mathbf{A}^+]\rangle$  and  $\mathbf{M}' = \langle[i\dot{\mathbf{A}}, \mathbf{A}^+]\rangle$ , using Zubarev's notation.<sup>18</sup> We get

$$\chi^{+-}(\mathbf{q}, \omega) = -\frac{M_{\mathbf{q}}^{(1)}}{\omega^2 - \omega_{\mathbf{q}}^2}. \quad (2)$$

The spectral moment  $M_{\mathbf{q}}^{(1)} = \langle [i\dot{S}_{\mathbf{q}}^+, S_{-\mathbf{q}}^-] \rangle$  is given by

$$M_{\mathbf{q}}^{(1)} = -4C_{1,0,0}(1 - \cos q_x) - 4R_y C_{0,1,0}(1 - \cos q_y) - 4R_z C_{0,0,1}(1 - \cos q_z). \quad (3)$$

The two-spin correlation functions  $C_{\mathbf{r}} = \langle S_0^+ S_{\mathbf{r}}^- \rangle \equiv C_{n,m,l}$  with  $\mathbf{r} = n\mathbf{e}_x + m\mathbf{e}_y + l\mathbf{e}_z$  are calculated from

$$C_{\mathbf{r}} = \frac{1}{N} \sum_{\mathbf{q}} C_{\mathbf{q}} e^{i\mathbf{qr}} \quad , \quad C_{\mathbf{q}} = \frac{M_{\mathbf{q}}^{(1)}}{2\omega_{\mathbf{q}}} [1 + 2n(\omega_{\mathbf{q}})], \quad (4)$$

where  $n(\omega_{\mathbf{q}}) = (e^{\omega_{\mathbf{q}}/T} - 1)^{-1}$ . The NN correlation functions are directly related to the internal energy per site by  $\epsilon = \frac{3}{2}(C_{1,0,0} + R_y C_{0,1,0} + R_z C_{0,0,1})$ .

To obtain the spectrum in the approximation  $-\ddot{S}_{\mathbf{q}}^+ = \omega_{\mathbf{q}}^2 S_{\mathbf{q}}^+$ , we take the site representation and decouple the products of three spin operators in  $-\ddot{S}_i^+$  along NN sequences introducing vertex parameters in the spirit of the scheme proposed by Shimahara and Takada<sup>19</sup> and extending the decoupling given in Ref. 17,

$$S_i^+ S_j^+ S_l^- = \alpha_1^{x,y,z} \langle S_j^+ S_l^- \rangle S_i^+ + \alpha_2 \langle S_i^+ S_l^- \rangle S_j^+. \quad (5)$$

Here  $\alpha_1^x$ ,  $\alpha_1^y$ , and  $\alpha_1^z$  are attached to NN correlation functions along the  $x$ -,  $y$ - and  $z$ -directions, respectively, and  $\alpha_2$  is associated with the longer ranged correlation functions. We obtain

$$\begin{aligned} \omega_{\mathbf{q}}^2 = & 1 + R_y^2 + R_z^2 - \cos q_x - R_y^2 \cos q_y - R_z^2 \cos q_z + 2\alpha_1^x C_{1,0,0} \cos(2q_x) - 2\alpha_2 C_{2,0,0} \cos q_x \\ & + 2R_y^2 (\alpha_1^y C_{0,1,0} \cos(2q_y) - \alpha_2 C_{0,2,0} \cos q_y) + 2R_z^2 (\alpha_1^z C_{0,0,1} \cos(2q_z) - \alpha_2 C_{0,0,2} \cos q_z) \\ & - 2\alpha_1^x C_{1,0,0} \cos q_x + 2\alpha_2 C_{2,0,0} - 2R_y^2 (\alpha_1^y C_{0,1,0} \cos q_y - \alpha_2 C_{0,2,0}) - 2R_z^2 (\alpha_1^z C_{0,0,1} \cos q_z - \alpha_2 C_{0,0,2}) \\ & + 4R_y ((\alpha_1^x C_{1,0,0} + \alpha_1^y C_{0,1,0}) \cos q_x \cos q_y - \alpha_2 C_{1,1,0} (\cos q_x + \cos q_y)) \\ & + 4R_z ((\alpha_1^x C_{1,0,0} + \alpha_1^z C_{0,0,1}) \cos q_x \cos q_z - \alpha_2 C_{1,0,1} (\cos q_x + \cos q_z)) \\ & + 4R_y R_z ((\alpha_1^y C_{0,1,0} + \alpha_1^z C_{0,0,1}) \cos q_y \cos q_z - \alpha_2 C_{0,1,1} (\cos q_y + \cos q_z)) \\ & - 4R_y (\alpha_1^x C_{1,0,0} \cos q_y + \alpha_1^y C_{0,1,0} \cos q_x - 2\alpha_2 C_{1,1,0}) - 4R_z (\alpha_1^x C_{1,0,0} \cos q_z + \alpha_1^z C_{0,0,1} \cos q_x - 2\alpha_2 C_{1,0,1}) \\ & - 4R_y R_z (\alpha_1^y C_{0,1,0} \cos q_z + \alpha_1^z C_{0,0,1} \cos q_y - 2\alpha_2 C_{0,1,1}). \end{aligned} \quad (6)$$

Note that our scheme preserves the rotational symmetry in spin space, i.e.  $\chi^{zz}(\mathbf{q}, \omega) \equiv \chi(\mathbf{q}, \omega) = \frac{1}{2}\chi^{+-}(\mathbf{q}, \omega)$ . For  $|\mathbf{q}| \ll 1$  we have

$$\omega_{\mathbf{q}}^2 = c_x^2 q_x^2 + c_y^2 q_y^2 + c_z^2 q_z^2, \quad (7)$$

with the squared spin-wave velocities

$$c_x^2 = \frac{1}{2} - 3\alpha_1^x C_{1,0,0} + \alpha_2 C_{2,0,0} - 2R_y(\alpha_1^x C_{1,0,0} - \alpha_2 C_{1,0,0}) - 2R_z(\alpha_1^x C_{1,0,0} - \alpha_2 C_{1,0,1}), \quad (8)$$

$$c_y^2 = R_y^2 \left( \frac{1}{2} - 3\alpha_1^y C_{0,1,0} + \alpha_2 C_{0,2,0} \right) - 2R_y(\alpha_1^y C_{0,1,0} - \alpha_2 C_{1,1,0}) - 2R_y R_z (\alpha_1^y C_{0,1,0} - \alpha_2 C_{0,1,1}), \quad (9)$$

and

$$c_z^2 = R_z^2 \left( \frac{1}{2} - 3\alpha_1^z C_{0,0,1} + \alpha_2 C_{0,0,2} \right) - 2R_z(\alpha_1^z C_{0,0,1} - \alpha_2 C_{1,0,1}) - 2R_y R_z (\alpha_1^z C_{0,0,1} - \alpha_2 C_{0,1,1}). \quad (10)$$

Considering the uniform static spin susceptibility  $\chi = \lim_{\mathbf{q} \rightarrow 0} M_{\mathbf{q}}^{(1)} / (2\omega_{\mathbf{q}}^2)$ , the ratio of the anisotropic functions  $M_{\mathbf{q}}^{(1)}$  and  $\omega_{\mathbf{q}}^2$  must be isotropic in the limit  $\mathbf{q} \rightarrow 0$ . That is, the conditions

$$(c_y/c_x)^2 = R_y C_{0,1,0} / C_{1,0,0} \quad (11)$$

and

$$(c_z/c_x)^2 = R_z C_{0,0,1} / C_{1,0,0} \quad (12)$$

have to be fulfilled.

The critical behavior of the model (1) is reflected in our theory by the closure of the spectrum gap at  $\mathbf{Q} = (\pi, \pi, \pi)$  as  $T$  approaches  $T_N$  from above, so that  $\lim_{T \rightarrow T_N} \chi^{-1}(\mathbf{Q}) = 0$ . At  $T \leq T_N$  we have  $\omega_{\mathbf{Q}} = 0$  and, separating the condensation part  $C$ ,

$$C_{\mathbf{r}} = \frac{1}{N} \sum_{\mathbf{q}(\neq \mathbf{Q})} C_{\mathbf{q}} e^{i\mathbf{qr}} + C e^{i\mathbf{Qr}}, \quad (13)$$

where  $C$  results from (13) with  $\mathbf{r} = 0$  employing the sum rule  $C_{0,0,0} = \frac{1}{2}$ . Then the staggered magnetization  $m$  is calculated as

$$m^2 = \frac{1}{N} \sum_{\mathbf{r}} \langle \mathbf{S}_0 \mathbf{S}_{\mathbf{r}} \rangle e^{-i\mathbf{Qr}} = \frac{3}{2} C. \quad (14)$$

The theory has 14 quantities to be determined self-consistently (9 correlation functions in  $\omega_{\mathbf{q}}^2$ ,  $m$ , and 4 vertex parameters) and 13 self-consistency equations (10 Eqs. (13) including  $C_{0,0,0} = \frac{1}{2}$ , the LRO condition  $\omega_{\mathbf{Q}} = 0$ , and Eqs. (11) and (12)). If there is no LRO, we have  $\omega_{\mathbf{Q}} > 0$ , and the number of quantities and equations is reduced by one. As an additional condition for determining the free  $\alpha$  parameter at  $T = 0$ , we adjust the ground-state energy per site which we compose approximately as  $\epsilon(R_y, R_z) = \epsilon(R_y, 0) + \epsilon(0, R_z) - \epsilon(0, 0)$ , where  $\epsilon(R_y, 0)$  (and  $\epsilon(0, R_z)$ ) is taken from the Ising-expansion results by Affleck et al. for the 2D spatially anisotropic Heisenberg model,<sup>20</sup> and  $\epsilon(0, 0) = -0.4431$  is the Bethe-ansatz value. This approximation is suggested to be good at least for  $R_z \ll R_y$  (or  $R_y \ll R_z$ ).

To get an additional condition also at finite temperatures, where  $\epsilon$  data are not available and all vertex parameters are temperature dependent, we assume, following Refs. 19 and 16, the ratio

$$r_\alpha(T) \equiv \frac{\alpha_2(T) - 1}{\alpha_1^x(T) - 1} = r_\alpha(0) \quad (15)$$

as temperature independent.

### III. GROUND-STATE PROPERTIES

In Fig. 1 our results for the zero-temperature staggered magnetization  $m_0 \equiv m(T = 0)$  as a function of  $R_y$  and  $R_z$  are shown. They indicate an order-disorder transition at the phase boundary  $R_{z,c}(R_y)$  or  $R_{y,c}(R_z)$  (cf. inset). For  $R_z = 0$  we get the critical ratio  $R_{y,c}(0) \simeq 0.24$  which was already found in Ref. 17. In that paper the suppression of LRO below the finite value of  $R_{y,c}$  was interpreted, in combination with ED data, as indication of a rather sharp crossover in the spatial dependence of the spin correlation functions in the LRO phase at the coupling ratio  $R_{y,0} \simeq 0.2$ . The finite value of  $R_{y,c}$ , however, seems to be due to the approximations in our theory, since there are strong indications for  $R_{y,c} = 0$  (see Ref. 14). Accordingly, we cannot explain the tiny magnetic moments of  $\text{Sr}_2\text{CuO}_3$  and  $\text{Ca}_2\text{CuO}_3$ ,<sup>2</sup> since for  $R_y \ll 1$ ,<sup>3</sup> we have  $m = 0$ . This result is just opposite to the overestimation of  $m$  by all previous spin-wave theories. As seen in the phase diagram (inset of Fig. 1), the inclusion of the interplane coupling  $R_z$  stabilizes the LRO, where this effect is quite considerable even at very small values of  $R_z$ .

Figure 2 exhibits some short-ranged spin correlation functions at  $T = 0$ . For  $R_z = 0$ , in Ref. 17 the correlators  $C_{1,0,0}, C_{0,1,0}$ , and  $C_{1,1,0}$  as functions of  $R_y$  were found to agree well with the ED data. For  $R_z = 0.02$  (cf. Fig. 2) our results deviate only slightly from those at  $R_z = 0$ . The sign changes and magnitudes of  $C_r$  reflect the AFM SRO. In the limit  $R_y \rightarrow 0$  the correlations between the  $x$ - $z$ -planes vanish. At  $R_z > R_{z,c}(0) \simeq 0.24$  the LRO enhances the inter- $x$ - $z$  plane correlators and results in their sharp drop towards their limiting value  $C e^{i\mathbf{Q}\mathbf{r}}$  as  $R_y \rightarrow 0$ . This is visible in the data for  $R_z = 0.35$  in Fig. 2.

### IV. FINITE-TEMPERATURE RESULTS

At nonzero temperatures we have solved the self-consistency equations (13) supplemented by the conditions (11), (12), and (15) to obtain the magnetization  $m(T)$ , the Néel temperature ( $m(T_N) = 0$ ), the static spin susceptibility, and the anisotropic correlation lengths.

In Fig. 3 the Néel temperature is plotted as a function of  $R_z$ . For  $R_z = 0$  we get  $T_N = 0$  (see Ref. 16), in agreement with the Mermin-Wagner theorem. The increase of  $T_N$  with  $R_z$  is governed by the intra- $x$ - $y$  plane anisotropy. At a fixed value of  $R_z$ , the decrease of  $T_N$  with decreasing  $R_y$  is in accordance with the reduced zero-temperature magnetization (cf. Fig. 1). Comparing our results for  $R_y = 1$  with previous RPA/mean-field approaches (see Table I), we ascribe the reduction of  $T_N$  as compared with Refs. 6,8, and 12 to the improved description of SRO. That is, the LRO is suppressed in favor of a paramagnetic phase with pronounced AFM SRO. If  $R_z$  is fit to the Néel temperatures of real systems, the strong overestimation of  $T_N$  by previous theories results in very small values of the interplane coupling. In our approach the resulting  $R_z$  values turn out to be higher. Considering  $\text{La}_2\text{CuO}_4$  with  $T_N = 325\text{K}^{9,21}$  and putting  $J = 130\text{meV}$  ( $J \equiv J_x = J_y$ ) or  $J = 117\text{meV}^{16}$  we obtain  $R_z \simeq 10^{-3}$  or  $R_z \simeq 1.6 \times 10^{-3}$ , respectively, in contrast to  $R_z < 10^{-4}$  according to Refs. 6 and 12. For  $\text{Ca}_{0.85}\text{Sr}_{0.15}\text{CuO}_2$  ( $T_N = 540\text{K}$ ,  $J = 125\text{meV}^{22}$ ) we get  $R_z \simeq 1.2 \times 10^{-2}$  as compared with  $R_z \simeq 2.5 \times 10^{-2}$  obtained from a fit of the low-temperature magnetization data.<sup>22</sup>

Figure 4 shows the temperature dependence of the staggered magnetization at  $R_y = 1$  (for the zero-temperature values, compare with Fig. 1). The shape of the normalized curve  $m/m_0$  versus  $T/T_N$  (see inset) depends on the single parameter  $R_z$  and is similar to that found in previous spin-wave theories.<sup>6–8,10</sup> At low enough temperatures the system exhibits 3D behavior, so that the decrease of  $m$  follows a  $T^2$  law. This was also observed by NMR experiments on  $\text{La}_2\text{CuO}_4^{11}$  ( $T_N = 312\text{K}$ ) yielding  $m/m_0 = 1 - a(T/T_N)^2$  with  $a = 0.67$  for  $T \lesssim 100\text{K}$ . The NMR data is indicated in the inset of Fig. 4 (marked by a bold curve) and agrees well with our theory for  $R_z = 10^{-3}$  (as estimated above). For temperatures close to  $T_N$  our numerical results for  $m(T)$  are described by the law  $m(T) \propto (1 - T/T_N)^{1/2}$ . The square-root temperature behavior agrees with the findings of Refs. 7,8,10, and with the neutron scattering data on  $\text{La}_2\text{CuO}_4$ ,<sup>9</sup> but contradicts the result of Ref. 13 ( $m \propto 1 - T/T_N$ ).

Considering the AFM correlation lengths above  $T_N$  and for  $R_y = 1$ , the expansion of  $\chi(\mathbf{q})$  around  $\mathbf{Q}$ ,  $\chi(\mathbf{q}) = \chi(\mathbf{Q}) [1 + \xi_{xy}^2(k_x^2 + k_y^2) + \xi_z^2 k_z^2]^{-1}$  with  $\mathbf{k} = \mathbf{q} - \mathbf{Q}$ , yields the intraplane correlation length

$$\begin{aligned} \xi_{xy}^2 = -\omega_{\mathbf{Q}}^{-2} & \left[ \frac{1}{2} + 11\alpha_1^x C_{1,0,0} + \alpha_2 (C_{2,0,0} + 2C_{1,1,0}) + \right. \\ & \left. + 2R_z (\alpha_1^x C_{1,0,0} + 2\alpha_1^z C_{0,0,1} + \alpha_2 C_{1,0,1}) \right] - \frac{2C_{1,0,0}}{M_{\mathbf{Q}}^{(1)}} \end{aligned} \quad (16)$$

and the interplane correlation length

$$\xi_z^2 = -R_z \omega_{\mathbf{Q}}^{-2} [4(2\alpha_1^x C_{1,0,0} + \alpha_1^z C_{0,0,1} + \alpha_2 C_{1,0,1}) +$$

$$+R_z \left( \frac{1}{2} + 5\alpha_1^z C_{0,0,1} + \alpha_2 C_{0,0,2} \right) \right] - \frac{2R_z C_{0,0,1}}{M_{\mathbf{Q}}^{(1)}} . \quad (17)$$

In Fig. 5 the influence of the interplane coupling on the temperature dependence of  $\xi_{xy}^{-1}$  and  $\xi_z^{-1}$  (inset) is shown. For comparison, the intraplane correlation length at  $R_z = 0$  (see also Ref. 16) is plotted, where the low-temperature expansion  $\xi_{xy} = 2(2\alpha_1^x |C_{1,0,0}(0)|)^{1/2} T^{-1} \exp[2\pi\alpha_1^x m_0^2/(3T)]$  holds up to  $T = 0.2$  within a deviation of about 6% from the full temperature dependence calculated by Eq.(16). For  $R_z > 0$  the correlation lengths diverge at  $T_N$ , since the gap  $\omega_{\mathbf{Q}}$  closes as  $T$  approaches  $T_N$  from above. In the vicinity of  $T_N$ ,  $\xi_{xy}^{-1}$  and  $\xi_z^{-1}$  behave as  $T - T_N$  also found by previous mean-field approaches.<sup>12,13</sup>

Let us compare our results for the intraplane correlation length with the neutron-scattering data on La<sub>2</sub>CuO<sub>4</sub><sup>21</sup> in the range 340K  $\leq T \leq$  820K shown in Fig. 6. Taking  $J$  as obtained previously<sup>16</sup> from a least-squares fit of  $\xi_{xy}$  in the 2D model ( $a = 3.79\text{\AA}$ ),  $J = 117\text{meV}$ , for  $T > 500\text{K}$  and  $R_z \lesssim 3.5 \times 10^{-3}$  we get a good quantitative agreement with experiments. In Ref. 16 the deviation of the theory for  $R_z = 0$  and  $T < 500\text{K}$  from the experimental data was ascribed to the appearance of the preexponential factor  $T^{-1}$  in the low-temperature expansion of  $\xi_{xy}$  which is an artifact of our mean-field approach. However, this deviation may be reduced by the inclusion of the interplane coupling, since  $\xi_{xy}^{-1}(T_N) = 0$ . For  $T_N = 325\text{K}$ <sup>21</sup> we get  $R_z \simeq 1.6 \times 10^{-3}$  (see above, Fig. 3), and the theoretical  $\xi_{xy}^{-1}$  curve lies between the  $R_z = 0$  result and the experiments. The discrepancy between the theoretical and experimental low-temperature correlation lengths may be further reduced by the choice of higher  $R_z$  values. Taking, for example,  $R_z = 3.4 \times 10^{-3}$ , we get a very good quantitative agreement (cf. Fig. 6) down to 360K; however, the Néel temperature turns out to be somewhat higher ( $T_N = 353\text{K}$ ).

Finally, we consider the uniform static spin susceptibility  $\chi(T) = \lim_{\mathbf{q} \rightarrow \mathbf{0}} \chi(\mathbf{q})$ . In Fig. 7 the anisotropy effects on the temperature dependence are demonstrated. For  $R_z = 0$  and a strong intraplane anisotropy ( $R_y < 0.2$ ) the minimum of  $\chi(T)$  at a finite temperature, being an artifact of our approach, may signal the crossover in the spatial dependence of the spin correlation functions at  $R_{y,0} \simeq 0.2$  as was discussed in Sec. III. Note that such a minimum in the 1D model ( $R_y = 0$ ) was also found in Ref. 23. At  $R_y > 0.2$ , the increase of  $\chi$  with temperature, the maximum at  $T_{max}$  near the exchange energy  $J_x = 1$  (see inset), and the crossover to the high-temperature Curie-Weiss behavior are due to the decrease of AFM SRO with increasing temperature (cf. Ref. 16). Let us point out that the susceptibility maximum is totally missed in RPA theories.<sup>7</sup> With increasing  $R_y$ , we obtain an increase of  $T_{max}$  which agrees with a general tendency found in various spin-1/2 Heisenberg models and analyzed in Ref. 5. For comparison, the exact values at  $R_y = 0$  and  $R_y = 1$  are given by  $T_{max} = 0.64$ <sup>24</sup> and  $T_{max} = 0.94$ ,<sup>25</sup> respectively. Since our theory allows the calculation of  $T_{max}$  at any spatial anisotropy, it may provide a reliable interpretation

of experimental data on low-dimensional spin systems. Considering the maximum spin susceptibility  $\chi_{max} = \chi(T_{max})$ , again our results are in accordance with the general behavior:<sup>5</sup>  $\chi_{max}$  increases with decreasing  $T_{max}$ , i.e. with decreasing  $R_y$ . Concerning the influence of the interplane coupling, the enhancement of the low-temperature susceptibility by  $R_z$  may be explained by the weakening of the SRO effect in higher dimensions. As seen from Figs. 7 and 3, the uniform susceptibility has no singularity at the Néel temperature, contrary to the RPA result of Ref. 7 revealing a peak of  $\chi(T)$  at  $T_N$ . Concerning the maximum in  $\chi(T)$  of La<sub>2</sub>CuO<sub>4</sub>, we get  $T_{max} = 1.19J = 1615\text{K}$  (cf. Fig. 7,  $J = 117\text{meV}$ ). This value roughly agrees with the estimate given by Johnston,<sup>26</sup>  $T_{max} = 1460\text{K}$ , by means of a scaling analysis of the susceptibility data below 800K.

## V. SUMMARY

In this paper we have extended the spin-rotation-invariant Green's-function theory of magnetic LRO and SRO in 2D Heisenberg models<sup>16,17</sup> to the 3D Heisenberg antiferromagnet with arbitrary spatial anisotropy. Our theory provides a satisfactory interpolation between the low-temperature and high-temperature behavior, where the temperature dependent SRO, described in term of two-spin correlation functions, is adequately taken into account. The main results are summarized as follows.

- (i) The incorporation of SRO results in a strong suppression of Néel order with increasing anisotropy and in a reduced Néel temperature as compared with previous spin-wave approaches.
- (ii) The temperature dependence of the uniform static spin susceptibility reveals a maximum in the short-range ordered paramagnetic phase and a crossover to the Curie-Weiss law. The position of the maximum is influenced by the spatial anisotropy.
- (iii) Comparing the theory with experiments on the magnetization and correlation length of La<sub>2</sub>CuO<sub>4</sub>, a good quantitative agreement is found.

From the results of our theory we conclude that the application of this approach to extended Heisenberg models (anisotropy in spin space, frustration) may be promising to describe the SRO effects on the unconventional magnetic properties of real low-dimensional spin systems.

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**TABLE I.** Néel temperature  $T_N/J_x$  at  $R_y = 1$  compared with other approaches

$-\log_{10}(R_z)$	Fig. 3	Ref. 6	Ref. 8	Ref. 12
4	0.17	0.48	0.29	0.25
3	0.22	0.65	0.38	0.34
2	0.36	0.80	0.54	0.47
1	0.56	1.15		0.68

## Figures

Fig. 1. Staggered magnetization at  $T = 0$  as a function of spatial anisotropy. The inset shows the stability region of Néel order.

Fig. 2. Spin correlation functions at  $T = 0$  for different spatial anisotropies.

Fig. 3. Néel temperature as a function of  $R_z = J_z/J_x$ .

Fig. 4. Staggered magnetization vs. temperature for  $R_y = 1$ . The inset shows the  $R_z$  dependence of the normalized curves compared with the NMR data on  $\text{La}_2\text{CuO}_4$ <sup>11</sup> (bold curve).

Fig. 5. Inverse antiferromagnetic correlation lengths within ( $\xi_{xy}^{-1}$ ) and between the  $x$ - $y$  planes ( $\xi_z^{-1}$ , see inset) for  $R_y = 1$ .

Fig. 6. Inverse antiferromagnetic intraplane correlation length in  $\text{La}_2\text{CuO}_4$  obtained by the neutron-scattering experiments of Ref. 21 and from the theory ( $R_y = 1$ ) for different  $R_z$  values.

Fig. 7. Uniform static spin susceptibility vs.  $T$ . The inset exhibits the position  $T_{max}$  of the maximum in  $\chi(T)$  vs.  $R_y$ .













